

# The Maximal Matching Energy of Tricyclic Graphs

Lin Chen, Yongtang Shi\*

Center for Combinatorics and LPMC-TJKLC, Nankai University  
Tianjin 300071, P.R. China.

E-mail: chenlin1120120012@126.com, shi@nankai.edu.cn

(Received May 13, 2014)

## Abstract

Gutman and Wagner proposed the concept of the matching energy (ME) and pointed out that the chemical applications of ME go back to the 1970s. Let  $G$  be a simple graph of order  $n$  and  $\mu_1, \mu_2, \dots, \mu_n$  be the roots of its matching polynomial. The matching energy of  $G$  is defined to be the sum of the absolute values of  $\mu_i$  ( $i = 1, 2, \dots, n$ ). Gutman and Cvetkoić determined the tricyclic graphs on  $n$  vertices with maximal number of matchings by a computer search for small values of  $n$  and by an induction argument for the rest. Based on this result, in this paper, we characterize the graphs with the maximal value of matching energy among all tricyclic graphs, and completely determine the tricyclic graphs with the maximal matching energy. We prove our result by using Coulson-type integral formula of matching energy, which is similar as the method to comparing the energies of two quasi-order incomparable graphs.

## 1 Introduction

In this paper, all graphs under our consideration are finite, connected, undirected and simple. For more notations and terminologies that will be used in the sequel, we refer to [2]. Let  $G$  be such a graph, and let  $n$  and  $m$  be the number of its vertices and

---

\*The corresponding author.

edges, respectively. A *matching* in a graph  $G$  is a set of pairwise nonadjacent edges. A matching  $M$  is called a  $k$ -*matching* if the size of  $M$  is  $k$ . Denote by  $m(G, k)$  the number of  $k$ -matchings of  $G$ , where  $m(G, 1) = m$  and  $m(G, k) = 0$  for  $k > \lfloor \frac{n}{2} \rfloor$  or  $k < 0$ . In addition, define  $m(G, 0) = 1$ . The matching polynomial of graph  $G$  is defined as

$$\alpha(G) = \alpha(G, x) = \sum_{k \geq 0} (-1)^k m(G, k) x^{n-2k}.$$

In 1977, Gutman [4] proposed the concept of graph energy. The energy of  $G$  is defined as the sum of the absolute values of its eigenvalues, namely,

$$E(G) = \sum_{i=1}^n |\lambda_i|,$$

where  $\lambda_1, \lambda_2, \dots, \lambda_n$  denote the eigenvalues of  $G$ . The theory of graph energy is well developed. The graph energy has been rather widely studied by theoretical chemists and mathematicians. For details, we refer the book on graph energy [24] and reviews [8, 10]. Recently, Gutman and Wagner [13] defined the matching energy of a graph  $G$  based on the zeros of its matching polynomial [3, 5].

**Definition 1.1** *Let  $G$  be a simple graph with order  $n$ , and  $\mu_1, \mu_2, \dots, \mu_n$  be the zeros of its matching polynomial. Then,*

$$ME(G) = \sum_{i=1}^n |\mu_i|. \quad (1.1)$$

Moreover, Gutman and Wagner [13] pointed out that the matching energy is a quantity of relevance for chemical applications. They arrived at the simple relation:

$$TRE(G) = E(G) - ME(G),$$

where  $TRE(G)$  is the so-called “topological resonance energy” of  $G$ . About the chemical applications of matching energy, for more details see [1, 11, 12].

An important tool of graph energy is the Coulson-type integral formula [4] (with regard to  $G$  be a tree  $T$ ):

$$E(T) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[ \sum_{k \geq 0} m(T, k) x^{2k} \right] dx, \quad (1.2)$$

which is valid for any tree  $T$  (or, more generally, for any forest). Being similar to Eq.(1.2), the matching energy also has a beautiful formula as follows [13].

**Proposition 1.2** *Let  $G$  be a simple graph of order  $n$ , and  $m(G, k)$  be the number of its  $k$ -matchings,  $k = 0, 1, 2, \dots, \lfloor \frac{n}{2} \rfloor$ . The matching energy of  $G$  is given by*

$$ME = ME(G) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[ \sum_{k \geq 0} m(G, k) x^{2k} \right] dx. \quad (1.3)$$

Combining Eq.(1.2) with Eq.(1.3), it immediately follows that: if  $G$  is a forest, then its matching energy coincides with its energy.

Formula (1.2) implies that the energy of a tree is a monotonically increasing function of any  $m(T, k)$ . In particular, if  $T'$  and  $T''$  are two trees for which  $m(T', k) \geq m(T'', k)$  holds for all  $k \geq 1$ , then  $E(T') \geq E(T'')$ . If, in addition,  $m(T', k) > m(T'', k)$  for at least one  $k$ , then  $E(T') > E(T'')$ . Obviously, by Formula (1.3) and the monotonicity of the logarithm function, the result is also valid for  $ME$ . Thus, we can define a *quasi-order* “ $\succeq$ ” as follows: If two graphs  $G_1$  and  $G_2$  have the same order and size, then

$$G_1 \succeq G_2 \iff m(G_1, k) \geq m(G_2, k) \quad \text{for } 1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor. \quad (1.4)$$

And if  $G_1 \succeq G_2$  we say that  $G_1$  is *m-greater than*  $G_2$  or  $G_2$  is *m-smaller than*  $G_1$ . If  $G_1 \succeq G_2$  and  $G_2 \succeq G_1$ , the graphs  $G_1$  and  $G_2$  are said to be *m-equivalent*, denote it by  $G_1 \sim G_2$ . If  $G_1 \succeq G_2$ , but the graphs  $G_1$  and  $G_2$  are not *m-equivalent* (i.e., there exists some  $k$  such that  $m(G_1, k) > m(G_2, k)$ ), then we say that  $G_1$  is *strictly m-greater than*  $G_2$ , write  $G_1 \succ G_2$ . If neither  $G_1 \succeq G_2$  nor  $G_2 \succeq G_1$ , the two graphs  $G_1$  and  $G_2$  are said to be *m-incomparable* and we denote this by  $G_1 \# G_2$ .

The relation  $\sim$  is an equivalence relation in any set of graphs  $\gamma$ . The corresponding equivalence classes will be called *matching equivalence classes* (of the set  $\gamma$ ). The relation  $\succeq$  induces a partial ordering of the set  $\gamma / \sim$ . An equivalence class is said to be the *greatest* if it is greater than any of other class. A class is *maximal* if there is no other class greater than it. The graphs belonging to greatest (resp. maximal)

matching equivalence classes will be said to be *m-greatest* (resp. *m-maximal*) in the set considered.

According to Eq.(1.3) and Eq.(1.4), we have

$$G_1 \succeq G_2 \implies ME(G_1) \geq ME(G_2)$$

and

$$G_1 \succ G_2 \implies ME(G_1) > ME(G_2).$$

It follows that the *m-greatest* graphs must have greatest matching energy, and the *m-maximal* graphs must have greater matching energy than other graphs not to be *m-maximal*.

A connected simple graph with  $n$  vertices and  $n$ ,  $(n + 1)$ ,  $(n + 2)$  edges are called *unicyclic*, *bicyclic*, *tricyclic graphs*, respectively. Denote by  $\mathcal{B}_n$  the set of all connected bicyclic graphs of order  $n$ , and by  $\mathcal{T}_n$  the set of all connected tricyclic graphs on  $n$  vertices. Let  $S_n^*$  denote the graph obtained by joining one pendant vertex of  $S_n$  to its other two pendant vertices, respectively. Similarly, let  $S_n^{**}$  be the graph obtained by joining one pendent vertex of  $S_n$  to its another three pendent vertices, respectively. Let  $K_4^{n-4}$  denote the graph obtained by attaching  $(n - 4)$  pendent vertices to one of the four vertices of  $K_4$ . Of course,  $S_n^{**}, K_4^{n-4} \in \mathcal{T}_n$  (as shown in Fig. 1.1). Denote by  $C_n$  the cycle graph of order  $n$  and  $P_n$  the path graph of order  $n$ , and let  $P_n^{k,\ell}$  be the graph obtained by connecting two cycles  $C_k$  and  $C_\ell$  with a path  $P_{n-k-\ell}$ .

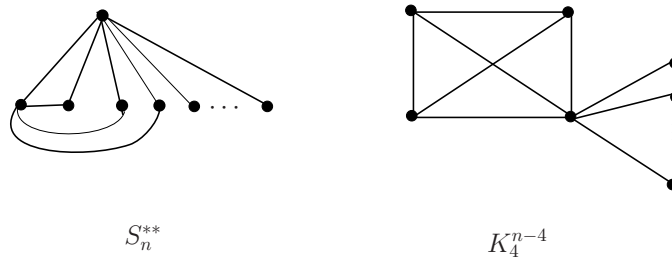


Figure 1.1: Tricyclic graphs with minimal matching energy.

As the research of extremal graph energy is an amusing work (for some newest literatures see [14–18, 22]), the study on extremal matching energy is also interesting.

In [13], the authors gave some elementary results on the matching energy and obtained that  $ME(S_n^+) \leq ME(G) \leq ME(C_n)$  for any unicyclic graph  $G$ , where  $S_n^+$  is the graph obtained by adding a new edge to the star  $S_n$ . In [20], Ji et al. proved that for  $G \in \mathcal{B}_n$  with  $n \geq 10$  and  $n = 8$ ,  $ME(S_n^*) \leq ME(G) \leq ME(P_n^{4,n-4})$ . In [19], the authors characterize the connected graphs (and bipartite graph) of order  $n$  having minimum matching energy with  $m$  ( $n + 2 \leq m \leq 2n - 4$ ) ( $n \leq m \leq 2n - 5$ ) edges. Especially, among all tricyclic graphs of order  $n \geq 5$ ,  $ME(G) \geq ME(S_n^{**})$ , with equality if and only if  $G \cong S_n^{**}$  or  $G \cong K_4^{n-4}$ . For more results on the matching energy, we refer to [21, 23]. In this paper, we characterize the graphs with the maximal matching energy among all tricyclic graphs, and completely determine the tricyclic graphs with the maximal matching energy.

## 2 Main Results

In the 1980s, Gutman determined the unicyclic [6], bicyclic [7], tricyclic [9] graphs with maximal matchings, i.e., graphs that are extremal with regard to the quasi-ordering  $\succeq$ . We introduce the result on tricyclic graphs, which will be used in our proof.

**Lemma 2.1** ([9]) *In the set of all tricyclic graphs with  $n$  vertices ( $n \geq 4$ ) the greatest matching equivalence class exists only for  $n = 4, 5, 6, 7, 8$  and 9. For  $n \geq 10$  there exist two maximal matching equivalence classes. All these equivalence classes possess a unique element, except for  $n = 9$ , when the number of  $m$ -greatest graph is two. The corresponding graphs are presented in Fig. 2.2.*

Our results are obtained based on the result of Lemma 2.1.

**Theorem 2.2** *Let  $G \in \mathcal{T}_n$  with  $n \geq 5$ . Then for  $n = 5$ ,  $ME(G) \leq ME(G^5)$ ; for  $n = 6$ ,  $ME(G) \leq ME(G^6)$ ; for  $n = 7$ ,  $ME(G) \leq ME(G^7)$ ; for  $n = 8$ ,  $ME(G) \leq ME(G^8)$ ; for  $n = 9$ ,  $ME(G) \leq ME(G_{(1)}^9) = ME(G_{(2)}^9)$ ; for  $n = 10$ ,  $ME(G) \leq ME(G_{(2)}^{10})$ ; for  $n = 11$ ,  $ME(G) \leq ME(G_{(2)}^{11})$ ; for  $n = 12$ ,  $ME(G) \leq ME(G_{(2)}^{12})$ ; for  $n = 13$ ,  $ME(G) \leq ME(G_{(2)}^{13})$ ; for  $n \geq 14$ ,  $ME(G) \leq ME(G_{(2)}^n)$ , with equality if and*

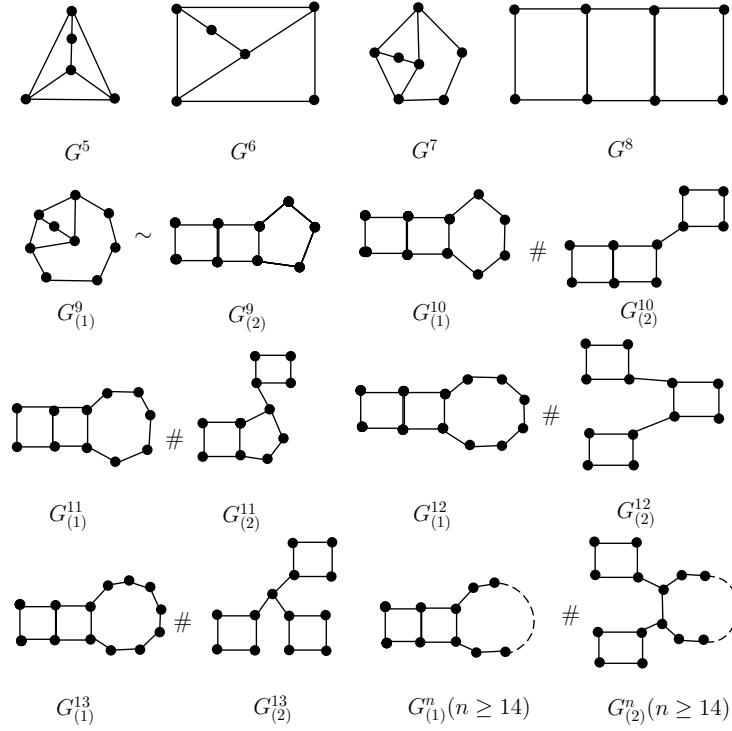


Figure 2.2: The tricyclic graphs with a maximal number of matchings.

only if  $G \cong G^n_{(2)}$ , where  $G^5, G^6, G^7, G^8, G^9_{(1)}, G^9_{(2)}, G^{10}_{(1)}, G^{10}_{(2)}, G^{11}_{(1)}, G^{11}_{(2)}, G^{12}_{(1)}, G^{12}_{(2)}, G^{13}_{(1)}, G^{13}_{(2)}, G^n_{(1)}, G^n_{(2)}$  are the graphs shown in Fig. 2.2.

We will prove our theorem by using Coulson-type integral formula of matching energy Eq.(1.3), which is similar as the method to comparing the energies of two quasi-order incomparable graphs [14–18, 22]. The following lemmas are needed.

**Lemma 2.3** ([25]) *For any real number  $X > -1$ , we have*

$$\frac{X}{1+X} \leq \ln(1+X) \leq X. \quad (2.1)$$

Let  $G$  be a simple graph. Let  $e$  be an edge of  $G$  connecting the vertices  $v_r$  and  $v_s$ . By  $G(e/j)$  we denote the graph obtained by inserting  $j$  ( $j \geq 0$ ) new vertices (of degree two) on the edge  $e$ . Hence if  $G$  has  $n$  vertices, then  $G(e/j)$  has  $n+j$  vertices; if  $j = 0$ , then  $G(e/j) = G$ ; if  $j > 0$ , then the vertices  $v_r$  and  $v_s$  are not adjacent in  $G(e/j)$ . There is such a result on the number of  $k$ -matchings of the graph  $G(e/j)$ .

**Lemma 2.4** ([9]) For all  $j \geq 0$ ,

$$m(G(e/j + 2), k) = m(G(e/j + 1), k) + m(G(e/j), k - 1).$$

We will divide Theorem 2.2 into the following two theorems according to the values of  $n$ .

**Theorem 2.5** Let  $G \in \mathcal{T}_n$  with  $n \geq 5$ . Then:

for  $n = 5$ ,  $ME(G) \leq ME(G^5)$ ; for  $n = 6$ ,  $ME(G) \leq ME(G^6)$ ; for  $n = 7$ ,  $ME(G) \leq ME(G^7)$ ; for  $n = 8$ ,  $ME(G) \leq ME(G^8)$ ; for  $n = 9$ ,  $ME(G) \leq ME(G_{(1)}^9) = ME(G_{(2)}^9)$ ; for  $n = 10$ ,  $ME(G) \leq ME(G_{(2)}^{10})$ ; for  $n = 11$ ,  $ME(G) \leq ME(G_{(2)}^{11})$ ; for  $n = 12$ ,  $ME(G) \leq ME(G_{(2)}^{12})$ ; for  $n = 13$ ,  $ME(G) \leq ME(G_{(2)}^{13})$ , where  $G^5, G^6, G^7, G^8, G_{(1)}^9, G_{(2)}^9, G_{(2)}^{10}, G_{(2)}^{11}, G_{(2)}^{12}, G_{(2)}^{13}$  are the graphs shown in Fig. 2.2. In each case, the equality holds if and only if  $G$  is isomorphic to the corresponding graph with maximal matching energy.

*Proof.* Let  $G$  be a graph in  $\mathcal{T}_n$  with  $n$  vertices.

For  $n = 5, 6, 7, 8$ , by Lemma 2.1,  $G^n$  is the  $m$ -greatest graph. We have known that the  $m$ -greatest graphs must have greatest matching energy. Hence if  $G \not\cong G^n$ , then  $ME(G) < ME(G^n)$ .

When  $n = 9$ ,  $G_{(1)}^9$  and  $G_{(2)}^9$  are  $m$ -equivalent, that is,  $m(G_{(1)}^9, k) = m(G_{(2)}^9, k)$  for all  $k$ . Then by Eq.(1.3), we have  $ME(G_{(1)}^9) = ME(G_{(2)}^9)$ . Moreover, if  $G \not\cong G_{(1)}^9$  and  $G \not\cong G_{(2)}^9$ , then  $ME(G) < ME(G_{(1)}^9) = ME(G_{(2)}^9)$  since  $(G_{(1)}^9 \sim G_{(2)}^9) \succ G$  by Lemma 2.1.

When  $n = 10$ , both  $G_{(1)}^{10}$  and  $G_{(2)}^{10}$  are  $m$ -maximal. Thus, if  $G \not\cong G_{(1)}^{10}$  and  $G \not\cong G_{(2)}^{10}$ , then  $ME(G) < ME(G_{(1)}^{10})$  as well as  $ME(G) < ME(G_{(2)}^{10})$ . In addition, we have  $m(G_{(1)}^{10}, 0) = 1$ ,  $m(G_{(1)}^{10}, 1) = 12$ ,  $m(G_{(1)}^{10}, 2) = 48$ ,  $m(G_{(1)}^{10}, 3) = 76$ ,  $m(G_{(1)}^{10}, 4) = 42$ ,  $m(G_{(1)}^{10}, 5) = 5$  and  $m(G_{(2)}^{10}, 0) = 1$ ,  $m(G_{(2)}^{10}, 1) = 12$ ,  $m(G_{(2)}^{10}, 2) = 48$ ,  $m(G_{(2)}^{10}, 3) = 75$ ,  $m(G_{(2)}^{10}, 4) = 42$ ,  $m(G_{(2)}^{10}, 5) = 6$ . Make use of Eq.(1.3), by computer-aided calculations, we get  $ME(G_{(1)}^{10}) = 13.8644$  and  $ME(G_{(2)}^{10}) = 13.9042$ . Therefore,  $ME(G) < ME(G_{(1)}^{10}) < ME(G_{(2)}^{10})$ .

For  $n = 11, 12, 13$ , both  $G_{(1)}^n$  and  $G_{(2)}^n$  are  $m$ -maximal. Similarly, by the help of computer, we get  $ME(G_{(1)}^{11}) = 14.9384$ ,  $ME(G_{(2)}^{11}) = 14.9466$ ,  $ME(G_{(1)}^{12}) = 16.3946$ ,  $ME(G_{(2)}^{12}) = 16.5052$ ,  $ME(G_{(1)}^{13}) = 17.5097$ ,  $ME(G_{(2)}^{13}) = 17.5678$ , respectively. Therefore, if  $G \not\cong G_{(2)}^n$ , then we have  $ME(G) \leq ME(G_{(1)}^n) < ME(G_{(2)}^n)$ .

The proof of the theorem is complete. ■

**Theorem 2.6** *Let  $G \in \mathcal{T}_n$  with  $n \geq 14$ . Then  $ME(G) \leq ME(G_{(2)}^n)$ , with equality if and only if  $G \cong G_{(2)}^n$ , where  $G_{(2)}^n$  is the graph shown in Fig. 2.2.*

*Proof.* By Lemma 2.1, both  $G_{(1)}^n$  and  $G_{(2)}^n$  are  $m$ -maximal. The  $m$ -maximal graphs must have greater matching energy than other graphs not to be  $m$ -maximal. Thus, if  $G \not\cong G_{(1)}^n$  and  $G \not\cong G_{(2)}^n$ , then  $ME(G) < ME(G_{(1)}^n)$  and  $ME(G) < ME(G_{(2)}^n)$ . It is sufficient to show that  $ME(G_{(1)}^n) < ME(G_{(2)}^n)$ . We will make full use of the definition of matching polynomial and Eq.(1.3).

Assume that  $|G(e/j + 2)| = n$ , then  $|G(e/j + 1)| = n - 1$  and  $|G(e/j)| = n - 2$ . According to Lemma 2.4, we have

$$\begin{aligned} \alpha(G(e/j + 2), x) &= \sum_{k \geq 0} (-1)^k m(G(e/j + 2), k) x^{n-2k} \\ &= \sum_{k \geq 0} (-1)^k m(G(e/j + 1), k) x^{n-2k} + \sum_{k \geq 0} (-1)^k m(G(e/j), k - 1) x^{n-2k} \\ &= x \sum_{k \geq 0} (-1)^k m(G(e/j + 1), k) x^{(n-1)-2k} \\ &\quad - \sum_{k \geq 0} (-1)^{k-1} m(G(e/j), k - 1) x^{(n-2)-2(k-1)} \\ &= x \alpha(G(e/j + 1), x) - \alpha(G(e/j), x). \end{aligned}$$

By the definition of  $G(e/j)$ , clearly,  $G_{(1)}^n = G_{(1)}(e/n - 7)$  and  $G_{(2)}^n = G_{(2)}(e/n - 11)$ , where  $G_{(1)}$  and  $G_{(2)}$  are the graphs shown in Fig. 2.3. Therefore, both  $\alpha(G_{(1)}^n, x)$  and  $\alpha(G_{(2)}^n, x)$  satisfy the recursive formula

$$f(n, x) = x f(n - 1, x) - f(n - 2, x).$$

The general solution of this linear homogeneous recurrence relation is

$$f(n, x) = C_1(x)(Y_1(x))^n + C_2(x)(Y_2(x))^n,$$



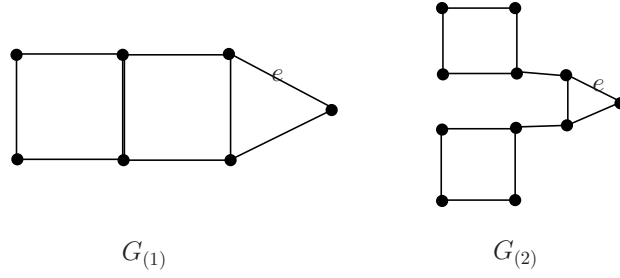


Figure 2.3: The fundamental graphs for constructing  $G_{(1)}^n$  and  $G_{(2)}^n$ .

where  $Y_1(x) = \frac{x+\sqrt{x^2-4}}{2}$ ,  $Y_2(x) = \frac{x-\sqrt{x^2-4}}{2}$ . By some elementary calculations, we can easily obtain the values of  $C_i(x)$  ( $i = 1, 2$ ) as follows.

In the following, we first consider  $\alpha(G_{(1)}^n, x)$ . It is easy to calculate the number of  $k$ -matchings of  $G_{(1)}$  and  $G_{(1)}(e/1)$ :  $m(G_{(1)}, 0) = 1$ ,  $m(G_{(1)}, 1) = 9$ ,  $m(G_{(1)}, 2) = 21$ ,  $m(G_{(1)}, 3) = 11$ ,  $m(G_{(1)}, k) = 0$  for  $k \geq 4$ ;  $m(G_{(1)}(e/1), 0) = 1$ ,  $m(G_{(1)}(e/1), 1) = 10$ ,  $m(G_{(1)}(e/1), 2) = 29$ ,  $m(G_{(1)}(e/1), 3) = 26$ ,  $m(G_{(1)}(e/1), 4) = 5$ ,  $m(G_{(1)}(e/1), k) = 0$  for  $k \geq 5$ . Then by Lemma 2.4, we can calculate the values of  $m(G_{(1)}(e/j), k)$  for all  $j \geq 2$  and  $k \geq 0$ . Thus, take the initial values as:

$$\begin{aligned}
\alpha(G_{(1)}(e/4), x) &= x^{11} - 13x^9 + 59x^7 - 114x^5 + 89x^3 - 21x \\
&= C_1(x)(Y_1(x))^{11} + C_2(x)(Y_2(x))^{11}; \\
\alpha(G_{(1)}(e/5), x) &= x^{12} - 14x^{10} + 71x^8 - 162x^6 + 165x^4 - 63x^2 + 5 \\
&= C_1(x)(Y_1(x))^{12} + C_2(x)(Y_2(x))^{12}.
\end{aligned}$$

It is easy to check that  $Y_1(x) + Y_2(x) = x$  and  $Y_1(x) \cdot Y_2(x) = 1$ . Therefore, by solving the two equalities above, we get

$$C_1(x) = \frac{Y_1(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}$$

and

$$C_2(x) = \frac{Y_2(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.$$

Define

$$\begin{aligned}
A_1(x) &= \frac{Y_1(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}, \\
A_2(x) &= \frac{Y_2(x)\alpha(G_{(1)}(e/5), x) - \alpha(G_{(1)}(e/4), x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.
\end{aligned}$$

Then we have  $\alpha(G_{(1)}^n, x) = A_1(x)(Y_1(x))^n + A_2(x)(Y_2(x))^n$ .

Now we consider  $\alpha(G_{(2)}^n, x)$ . Similarly, we get:  $m(G_{(2)}, 0) = 1$ ,  $m(G_{(2)}, 1) = 13$ ,  $m(G_{(2)}, 2) = 59$ ,  $m(G_{(2)}, 3) = 112$ ,  $m(G_{(2)}, 4) = 84$ ,  $m(G_{(2)}, 5) = 20$ ,  $m(G_{(2)}, k) = 0$  for  $k \geq 6$ ;  $m(G_{(2)}(e/1), 0) = 1$ ,  $m(G_{(2)}(e/1), 1) = 14$ ,  $m(G_{(2)}(e/1), 2) = 71$ ,  $m(G_{(2)}(e/1), 3) = 161$ ,  $m(G_{(2)}(e/1), 4) = 164$ ,  $m(G_{(2)}(e/1), 5) = 68$ ,  $m(G_{(2)}(e/1), 6) = 8$ ,  $m(G_{(2)}(e/1), k) = 0$  for  $k \geq 7$ . Then calculate the values of  $m(G_{(2)}(e/j), k)$  for all  $j \geq 2$  and  $k \geq 0$  by using Lemma 2.4. We can then take the initial values as:

$$\begin{aligned}\alpha(G_{(2)}, x) &= x^{11} - 13x^9 + 59x^7 - 112x^5 + 84x^3 - 20x \\ &= C_1(x)(Y_1(x))^{11} + C_2(x)(Y_2(x))^{11}; \\ \alpha(G_{(2)}(e/1), x) &= x^{12} - 14x^{10} + 71x^8 - 161x^6 + 164x^4 - 68x^2 + 8 \\ &= C_1(x)(Y_1(x))^{12} + C_2(x)(Y_2(x))^{12}.\end{aligned}$$

Therefore, we obtain that:

$$C_1(x) = \frac{Y_1(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}$$

and

$$C_2(x) = \frac{Y_2(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.$$

Define

$$\begin{aligned}B_1(x) &= \frac{Y_1(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_1(x))^{13} - (Y_1(x))^{11}}, \\ B_2(x) &= \frac{Y_2(x)\alpha(G_{(2)}(e/1), x) - \alpha(G_{(2)}, x)}{(Y_2(x))^{13} - (Y_2(x))^{11}}.\end{aligned}$$

Then we have  $\alpha(G_{(2)}^n, x) = B_1(x)(Y_1(x))^n + B_2(x)(Y_2(x))^n$ .

From the expression of  $\alpha(G, x)$ , we have

$$\alpha(G, ix) = \sum_{k \geq 0} (-1)^k m(G, k) (ix)^{n-2k} = i^n \sum_{k \geq 0} m(G, k) x^{n-2k} = (ix)^n \sum_{k \geq 0} m(G, k) x^{-2k},$$

where  $i^2 = -1$ . Thus, by Eq.(1.3), we get

$$\begin{aligned}
ME(G_{(1)}^n) - ME(G_{(2)}^n) &= \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[ \sum_{k \geq 0} m(G_{(1)}^n, k) x^{2k} \right] dx \\
&\quad - \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[ \sum_{k \geq 0} m(G_{(2)}^n, k) x^{2k} \right] dx \\
&= \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \frac{\sum_{k \geq 0} m(G_{(1)}^n, k) x^{2k}}{\sum_{k \geq 0} m(G_{(2)}^n, k) x^{2k}} dx \\
&= \frac{2}{\pi} \int_0^\infty \ln \frac{\sum_{k \geq 0} m(G_{(1)}^n, k) x^{-2k}}{\sum_{k \geq 0} m(G_{(2)}^n, k) x^{-2k}} dx \\
&= \frac{2}{\pi} \int_0^\infty \ln \frac{\alpha(G_{(1)}^n, ix)}{\alpha(G_{(2)}^n, ix)} dx \\
&= \frac{2}{\pi} \int_0^\infty \ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} dx.
\end{aligned} \tag{2.2}$$

By the definition of  $Y_1(x)$  and  $Y_2(x)$ , we have  $Y_1(ix) = \frac{x+\sqrt{x^2+4}}{2}i$  and  $Y_2(ix) = \frac{x-\sqrt{x^2+4}}{2}i$ . Now we define  $Z_1(x) = -iY_1(x) = \frac{x+\sqrt{x^2+4}}{2}$ ,  $Z_2(x) = -iY_2(x) = \frac{x-\sqrt{x^2+4}}{2}$ , and

$$f_1 = i\alpha(G_{(1)}(e/4), ix) = x^{11} + 13x^9 + 59x^7 + 114x^5 + 89x^3 + 21x$$

$$f_2 = \alpha(G_{(1)}(e/5), ix) = x^{12} + 14x^{10} + 71x^8 + 162x^6 + 165x^4 + 63x^2 + 5$$

$$g_1 = i\alpha(G_{(2)}, ix) = x^{11} + 13x^9 + 59x^7 + 112x^5 + 84x^3 + 20x$$

$$g_2 = \alpha(G_{(2)}(e/1), ix) = x^{12} + 14x^{10} + 71x^8 + 161x^6 + 164x^4 + 68x^2 + 8.$$

Then we have  $Y_1(ix) = iZ_1(x)$  and  $Y_2(ix) = iZ_2(x)$ . Moreover, It follows that

$$A_1(ix) = \frac{iZ_1(x)f_2 + if_1}{(iZ_1(x))^{13} - (iZ_1(x))^{11}} = \frac{Z_1(x)f_2 + f_1}{(Z_1(x))^{11}((Z_1(x))^2 + 1)}$$

$$A_2(ix) = \frac{iZ_2(x)f_2 + if_1}{(iZ_2(x))^{13} - (iZ_2(x))^{11}} = \frac{Z_2(x)f_2 + f_1}{(Z_2(x))^{11}((Z_2(x))^2 + 1)}$$

$$B_1(ix) = \frac{iZ_1(x)g_2 + ig_1}{(iZ_1(x))^{13} - (iZ_1(x))^{11}} = \frac{Z_1(x)g_2 + g_1}{(Z_1(x))^{11}((Z_1(x))^2 + 1)}$$

$$B_2(ix) = \frac{iZ_2(x)g_2 + ig_1}{(iZ_2(x))^{13} - (iZ_2(x))^{11}} = \frac{Z_2(x)g_2 + g_1}{(Z_2(x))^{11}((Z_2(x))^2 + 1)}.$$

Note that  $Y_1(ix) \cdot Y_2(ix) = 1$ ,  $Z_1(x) \cdot Z_2(x) = -1$ ,  $Z_1(x) + Z_2(x) = x$  and  $Z_{1(x)} - Z_2(x) = \sqrt{x^2 + 4}$ . We will distinguish with two cases.

**Case 1.**  $n$  is odd.

Now we have

$$\begin{aligned} & \ln \frac{A_1(ix)(Y_1(ix))^{n+2} + A_2(ix)(Y_2(ix))^{n+2}}{B_1(ix)(Y_1(ix))^{n+2} + B_2(ix)(Y_2(ix))^{n+2}} - \ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} \\ &= \ln \left( 1 + \frac{K_0(x)}{H_0(n, x)} \right), \end{aligned}$$

where

$$\begin{aligned} K_0(x) &= (A_1(ix)B_2(ix) - A_2(ix)B_1(ix))((Y_1(ix))^2 - (Y_2(ix))^2) = (f_2g_1 - f_1g_2)x \\ &= -x^{18} - 19x^{16} - 146x^{14} - 588x^{12} - 1342x^{10} - 1750x^8 - 1253x^6 - 460x^4 - 68x^2, \end{aligned}$$

and

$$\begin{aligned} H_0(n, x) &= (A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n)(B_1(ix)(Y_1(ix))^{n+2} + B_2(ix)(Y_2(ix))^{n+2}) \\ &= \alpha(G_{(1)}^n, ix) \cdot \alpha(G_{(2)}^{n+2}, ix) \\ &= \left( i^n \sum_{k \geq 0} m(G_{(1)}^n, k) x^{n-2k} \right) \left( i^{n+2} \sum_{k \geq 0} m(G_{(2)}^{n+2}, k) x^{n+2-2k} \right) \\ &= i^{2n+2} \left( \sum_{k \geq 0} m(G_{(1)}^n, k) x^{n-2k} \right) \left( \sum_{k \geq 0} m(G_{(2)}^{n+2}, k) x^{n+2-2k} \right). \end{aligned}$$

Obviously,  $K_0(x) < 0$ . Moreover, since  $n$  is odd, we have  $i^{2n+2} = 1$ , it follows that  $H_0(n, x)$  is a polynomial such that each term is of positive even degree of  $x$  and all coefficients are positive, i.e.,  $H_0(n, x) > 0$ . Hence,  $\frac{K_0(x)}{H_0(n, x)} < 0$ , which deduces that  $\ln(1 + \frac{K_0(x)}{H_0(n, x)}) < \ln 1 = 0$  for  $x > 0$  and odd  $n$ . So, the integrand of Eq.(2.2) is monotonically decreasing on  $n$ . Therefore, for  $n \geq 14$ ,

$$\int_0^\infty \ln \frac{\alpha(G_{(1)}^n, ix)}{\alpha(G_{(2)}^n, ix)} dx \leq \int_0^\infty \ln \frac{\alpha(G_{(1)}^{15}, ix)}{\alpha(G_{(2)}^{15}, ix)} dx = \int_0^\infty \ln \frac{\alpha(G_{(1)}(e/8), ix)}{\alpha(G_{(2)}(e/4), ix)} dx.$$

By computer-aided calculations, we get  $ME(G_{(1)}(e/8)) = 20.0728$  and  $ME(G_{(2)}(e/4)) = 20.1086$ . And then

$$\int_0^\infty \ln \frac{\alpha(G_{(1)}(e/8), ix)}{\alpha(G_{(2)}(e/4), ix)} dx = \frac{\pi}{2} (ME(G_{(1)}(e/8)) - ME(G_{(2)}(e/4))) = -0.05639 < 0.$$

So  $\int_0^\infty \ln \frac{\alpha(G_{(1)}^n, ix)}{\alpha(G_{(2)}^n, ix)} dx < 0$ . That is,

$$ME(G_{(1)}^n) - ME(G_{(2)}^n) = \frac{2}{\pi} \int_0^\infty \ln \frac{\alpha(G_{(1)}^n, ix)}{\alpha(G_{(2)}^n, ix)} dx < 0.$$

Therefore,  $ME(G_{(1)}^n) < ME(G_{(2)}^n)$  when  $n$  is odd.

**Case 2.**  $n$  is even.

Since  $x > 0$ , when  $n \rightarrow \infty$ , we have

$$\frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} \rightarrow \frac{A_1(ix)}{B_1(ix)}.$$

Then we have

$$\ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} - \ln \frac{A_1(ix)}{B_1(ix)} = \ln \left( 1 + \frac{K_1(n, x)}{H_1(n, x)} \right),$$

where

$$\begin{aligned} K_1(n, x) &= A_2(ix) \cdot B_1(ix) \cdot (Y_2(ix))^n - A_1(ix) \cdot B_2(ix) \cdot (Y_2(ix))^n \\ &= \frac{(f_2 g_1 - f_1 g_2)(Z_2(x))^n}{\sqrt{x^2 + 4}} \cdot i^n \\ &= \frac{(-x^{17} - 19x^{15} - 146x^{13} - 588x^{11} - 1342x^9 - 1750x^7 - 1253x^5 - 460x^3 - 68x)}{\sqrt{x^2 + 4}} \\ &\quad \cdot (Z_2(x))^n \cdot i^n, \end{aligned}$$

and

$$\begin{aligned} H_1(n, x) &= A_1(ix) \cdot B_1(ix) \cdot (Y_1(ix))^n + A_1(ix) \cdot B_2(ix) \cdot (Y_2(ix))^n \\ &= A_1(ix)(B_1(ix) \cdot (Y_1(ix))^n + B_2(ix) \cdot (Y_2(ix))^n) = A_1(ix)\alpha(G_{(2)}^n, ix) \\ &= i^n \cdot \frac{Z_1(x)f_2 + f_1}{(Z_1(x))^{11}((Z_1(x))^2 + 1)} \cdot \sum_{k \geq 0} m(G_{(2)}^n, k)x^{n-2k}. \end{aligned}$$

Since  $n$  is even,  $(Z_2(x))^n > 0$ . Hence  $K_1(n, x)/i^n$  is a polynomial of  $x$  with all coefficients being negative, namely, we always have  $K_1(n, x)/i^n < 0$ . On the other hand, since  $x > 0$ , we have  $Z_1(x) = \frac{x + \sqrt{x^2 + 4}}{2} > 0$ ,  $f_1 > 0$ ,  $f_2 > 0$  and  $m(G_{(2)}^n, k) > 0$  for all  $0 \leq k \leq \lfloor \frac{n}{2} \rfloor$ . Hence  $H_1(n, x)/i^n$  is a polynomial of  $x$  such that all the coefficients are positive. Therefore,  $\frac{K_1(n, x)}{H_1(n, x)} < 0$  for all  $x > 0$  and even  $n$ . Then  $\ln(1 + \frac{K_1(n, x)}{H_1(n, x)}) < \ln 1 = 0$ , i.e.,

$$\ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} < \ln \frac{A_1(ix)}{B_1(ix)}.$$

Thus, we have proved that the integrand of Eq.(2.2) is less than the corresponding limit function when  $n$  is even. Furthermore, since

$$1 + \frac{A_1(ix) - B_1(ix)}{B_1(ix)} = \frac{A_1(ix)}{B_1(ix)} = \frac{Z_1(x)f_2 + f_1}{Z_1(x)g_2 + g_1} > 0,$$

we have  $\frac{A_1(ix) - B_1(ix)}{B_1(ix)} > -1$ . Then by Lemma 2.3,  $\ln \frac{A_1(ix)}{B_1(ix)} \leq \frac{A_1(ix) - B_1(ix)}{B_1(ix)}$ . By some computer-aided calculations, we obtain that  $\int_0^\infty \frac{A_1(ix) - B_1(ix)}{B_1(ix)} dx = -0.09693$ . It means that

$$\int_0^\infty \ln \frac{A_1(ix)}{B_1(ix)} dx \leq \int_0^\infty \frac{A_1(ix) - B_1(ix)}{B_1(ix)} dx < 0.$$

Thus,

$$\begin{aligned} \frac{\pi}{2}(ME(G_{(1)}^n) - ME(G_{(2)}^n)) &= \int_0^\infty \ln \frac{A_1(ix)(Y_1(ix))^n + A_2(ix)(Y_2(ix))^n}{B_1(ix)(Y_1(ix))^n + B_2(ix)(Y_2(ix))^n} dx \\ &< \int_0^\infty \ln \frac{A_1(ix)}{B_1(ix)} dx < 0, \end{aligned}$$

i.e.,  $ME(G_{(1)}^n) < ME(G_{(2)}^n)$  when  $n$  is even.

Therefore, for all  $n \geq 14$ , we can always show that

$$ME(G_{(1)}^n) < ME(G_{(2)}^n),$$

the proof is thus complete. ■

**Acknowledgement.** The authors are very grateful to Professor Ivan Gutman for providing us with reference [9]. The authors are supported by NSFC, PCSIRT, China Postdoctoral Science Foundation (2014M551015) and China Scholarship Council.

## References

- [1] J. Aihara, A new definition of Dewar-type resonance energies, *J. Am. Chem. Soc.* **98**(1976) 2750–2758.
- [2] J.A. Bondy, U.S.R. Murty, *Graph Theory*, Springer, Berlin, 2008.
- [3] E.J. Farrell, An introduction to matching polynomials, *J. Combin. Theory B* **27**(1979) 75–86.

- [4] I. Gutman, Acyclic systems with extremal Hückel  $\pi$ -electron energy, *Theor. Chim. Acta* **45**(1977) 79–87.
- [5] I. Gutman, The matching polynomial, *MATCH Commun. Math. Comput. Chem.* **6**(1979) 75–91.
- [6] I. Gutman, Graphs with greatest number of matchings, *Publ. Inst. Math.*(Beograd) **27**(1980) 67–76.
- [7] I. Gutman, Correction of the paper “Graphs with greatest number of matchings”, *Publ. Inst. Math.*(Beograd) **32**(1982) 61–63.
- [8] I. Gutman, The Energy of a graph: Old and new results, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer, Berlin, 2001, pp. 196–211.
- [9] I. Gutman, D. Cvetković, Finding tricyclic graphs with a maximal number of matchings – another example of computer aided research in graph theory, *Publ. Inst. Math.*(Beograd) **35**(1984) 33–40.
- [10] I. Gutman, X. Li, J. Zhang, Graph energy, in: M. Dehmer, F. Emmert-Streib(Eds.), *Analysis of Complex Networks – From Biology to Linguistics*, Wiley-VCH, Weinheim, 2009, pp. 145–174.
- [11] I. Gutman, M. Milun, N. Trinajstić, Topological definition of delocalisation energy, *MATCH Commun. Math. Comput. Chem.* **1**(1975) 171–175.
- [12] I. Gutman, M. Milun, N. Trinajstić, Graph theory and molecular orbitals 19. Nonparametric resonance energies of arbitrary conjugated systems, *J. Am. Chem. Soc.* **99**(1977) 1692–1704.
- [13] I. Gutman, S. Wagner, The matching energy of a graph, *Discrete Appl. Math.* **160**(2012) 2177–2187.

- [14] B. Huo, S. Ji, X. Li, Y. Shi, Complete solution to a conjecture on the fourth maximal energy tree, *MATCH Commun. Math. Comput. Chem.* **66**(2011) 903–912.
- [15] B. Huo, S. Ji, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of bicyclic bipartite graphs, *Linear Algebra Appl.* **435**(2011) 804–810.
- [16] B. Huo, X. Li, Y. Shi, Complete solution to a conjecture on the maximal energy of unicyclic graphs, *European J. Combin.* **32**(2011) 662–673.
- [17] B. Huo, X. Li, Y. Shi, Complete solution to a problem on the maximal energy of unicyclic bipartite graphs, *Linear Algebra Appl.* **434**(2011) 1370–1377.
- [18] B. Huo, X. Li, Y. Shi, L. Wang, Determining the conjugated trees with the third-through the sixth-minimal energies, *MATCH Commun. Math. Comput. Chem.* **65**(2011) 521–532.
- [19] S. Ji, H. Ma, The extremal matching energy of graphs, *Ars Combin.*, accepted.
- [20] S. Ji, X. Li, Y. Shi, Extremal matching energy of bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **70**(2013) 697–706.
- [21] H. Li, Y. Zhou, L. Su, Graphs with extremal matching energies and prescribed parameters, *MATCH Commun. Math. Comput. Chem.* **72**(2014) 239–248.
- [22] J. Li, X. Li, Y. Shi, On the maximal energy tree with two maximum degree vertices, *Linear Algebra Appl.* **435**(2011) 2272–2284.
- [23] S. Li, W. Yan, The matching energy of graphs with given parameters, *Discrete Appl. Math.* **162**(2014) 415–420.
- [24] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [25] V. A. Zorich, *Mathematical Analysis*, MCCME, Moscow, 2002.